



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:15 am GMT

PDB ID : 3NIX  
Title : Crystal structure of flavoprotein/dehydrogenase from *Cytophaga hutchinsonii*.  
Northeast Structural Genomics Consortium Target Chr43.  
Authors : Vorobiev, S.; Su, M.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Foote, E.L.;  
Ciccosanti, C.; Maglaqui, M.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost,  
B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics  
Consortium (NESG)  
Deposited on : 2010-06-16  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

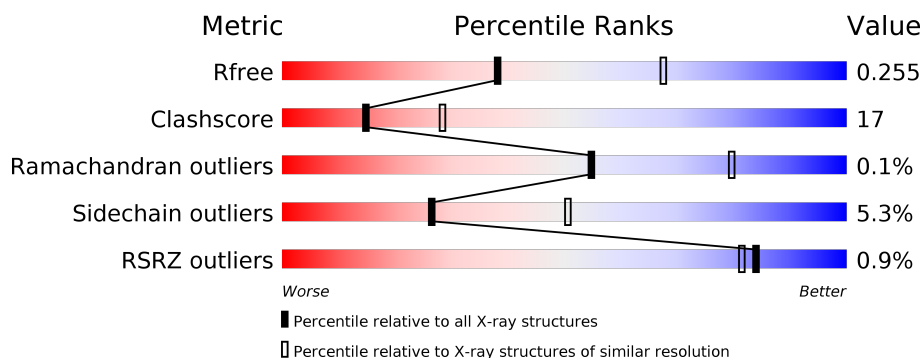
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	<div> <div>68%</div> <div>26%</div> <div>• •</div> </div>
1	B	421	<div> <div>%</div> <div>65%</div> <div>29%</div> <div>• 5%</div> </div>
1	C	421	<div> <div>%</div> <div>66%</div> <div>27%</div> <div>• •</div> </div>
1	D	421	<div> <div>%</div> <div>67%</div> <div>26%</div> <div>• •</div> </div>
1	E	421	<div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
1	F	421	<div> <div>%</div> <div>61%</div> <div>32%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	421	
1	H	421	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	F	506	X	-	-	-
2	FAD	G	507	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26852 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flavoprotein/dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	Se	0	0	0
			3210	2062	544	593	2	9			
1	B	400	Total	C	N	O	S	Se	0	0	0
			3162	2032	537	582	2	9			
1	C	405	Total	C	N	O	S	Se	0	0	0
			3185	2047	542	585	2	9			
1	D	403	Total	C	N	O	S	Se	0	0	0
			3183	2046	541	585	2	9			
1	E	406	Total	C	N	O	S	Se	0	0	0
			3212	2062	547	592	2	9			
1	F	402	Total	C	N	O	S	Se	0	0	0
			3182	2045	540	586	2	9			
1	G	406	Total	C	N	O	S	Se	0	0	0
			3204	2057	546	590	2	9			
1	H	403	Total	C	N	O	S	Se	0	0	0
			3177	2041	540	585	2	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	INITIATING METHIONINE	UNP Q11R94
A	414	LEU	-	EXPRESSION TAG	UNP Q11R94
A	415	GLU	-	EXPRESSION TAG	UNP Q11R94
A	416	HIS	-	EXPRESSION TAG	UNP Q11R94
A	417	HIS	-	EXPRESSION TAG	UNP Q11R94
A	418	HIS	-	EXPRESSION TAG	UNP Q11R94
A	419	HIS	-	EXPRESSION TAG	UNP Q11R94
A	420	HIS	-	EXPRESSION TAG	UNP Q11R94
A	421	HIS	-	EXPRESSION TAG	UNP Q11R94
B	1	MSE	-	INITIATING METHIONINE	UNP Q11R94
B	414	LEU	-	EXPRESSION TAG	UNP Q11R94
B	415	GLU	-	EXPRESSION TAG	UNP Q11R94
B	416	HIS	-	EXPRESSION TAG	UNP Q11R94

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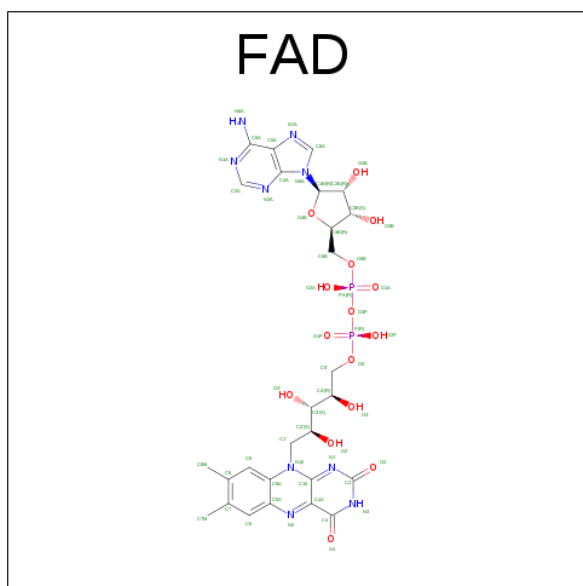
Chain	Residue	Modelled	Actual	Comment	Reference
B	417	HIS	-	EXPRESSION TAG	UNP Q11R94
B	418	HIS	-	EXPRESSION TAG	UNP Q11R94
B	419	HIS	-	EXPRESSION TAG	UNP Q11R94
B	420	HIS	-	EXPRESSION TAG	UNP Q11R94
B	421	HIS	-	EXPRESSION TAG	UNP Q11R94
C	1	MSE	-	INITIATING METHIONINE	UNP Q11R94
C	414	LEU	-	EXPRESSION TAG	UNP Q11R94
C	415	GLU	-	EXPRESSION TAG	UNP Q11R94
C	416	HIS	-	EXPRESSION TAG	UNP Q11R94
C	417	HIS	-	EXPRESSION TAG	UNP Q11R94
C	418	HIS	-	EXPRESSION TAG	UNP Q11R94
C	419	HIS	-	EXPRESSION TAG	UNP Q11R94
C	420	HIS	-	EXPRESSION TAG	UNP Q11R94
C	421	HIS	-	EXPRESSION TAG	UNP Q11R94
D	1	MSE	-	INITIATING METHIONINE	UNP Q11R94
D	414	LEU	-	EXPRESSION TAG	UNP Q11R94
D	415	GLU	-	EXPRESSION TAG	UNP Q11R94
D	416	HIS	-	EXPRESSION TAG	UNP Q11R94
D	417	HIS	-	EXPRESSION TAG	UNP Q11R94
D	418	HIS	-	EXPRESSION TAG	UNP Q11R94
D	419	HIS	-	EXPRESSION TAG	UNP Q11R94
D	420	HIS	-	EXPRESSION TAG	UNP Q11R94
D	421	HIS	-	EXPRESSION TAG	UNP Q11R94
E	1	MSE	-	INITIATING METHIONINE	UNP Q11R94
E	414	LEU	-	EXPRESSION TAG	UNP Q11R94
E	415	GLU	-	EXPRESSION TAG	UNP Q11R94
E	416	HIS	-	EXPRESSION TAG	UNP Q11R94
E	417	HIS	-	EXPRESSION TAG	UNP Q11R94
E	418	HIS	-	EXPRESSION TAG	UNP Q11R94
E	419	HIS	-	EXPRESSION TAG	UNP Q11R94
E	420	HIS	-	EXPRESSION TAG	UNP Q11R94
E	421	HIS	-	EXPRESSION TAG	UNP Q11R94
F	1	MSE	-	INITIATING METHIONINE	UNP Q11R94
F	414	LEU	-	EXPRESSION TAG	UNP Q11R94
F	415	GLU	-	EXPRESSION TAG	UNP Q11R94
F	416	HIS	-	EXPRESSION TAG	UNP Q11R94
F	417	HIS	-	EXPRESSION TAG	UNP Q11R94
F	418	HIS	-	EXPRESSION TAG	UNP Q11R94
F	419	HIS	-	EXPRESSION TAG	UNP Q11R94
F	420	HIS	-	EXPRESSION TAG	UNP Q11R94
F	421	HIS	-	EXPRESSION TAG	UNP Q11R94
G	1	MSE	-	INITIATING METHIONINE	UNP Q11R94

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Chain	Residue	Modelled	Actual	Comment	Reference
G	414	LEU	-	EXPRESSION TAG	UNP Q11R94
G	415	GLU	-	EXPRESSION TAG	UNP Q11R94
G	416	HIS	-	EXPRESSION TAG	UNP Q11R94
G	417	HIS	-	EXPRESSION TAG	UNP Q11R94
G	418	HIS	-	EXPRESSION TAG	UNP Q11R94
G	419	HIS	-	EXPRESSION TAG	UNP Q11R94
G	420	HIS	-	EXPRESSION TAG	UNP Q11R94
G	421	HIS	-	EXPRESSION TAG	UNP Q11R94
H	1	MSE	-	INITIATING METHIONINE	UNP Q11R94
H	414	LEU	-	EXPRESSION TAG	UNP Q11R94
H	415	GLU	-	EXPRESSION TAG	UNP Q11R94
H	416	HIS	-	EXPRESSION TAG	UNP Q11R94
H	417	HIS	-	EXPRESSION TAG	UNP Q11R94
H	418	HIS	-	EXPRESSION TAG	UNP Q11R94
H	419	HIS	-	EXPRESSION TAG	UNP Q11R94
H	420	HIS	-	EXPRESSION TAG	UNP Q11R94
H	421	HIS	-	EXPRESSION TAG	UNP Q11R94

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

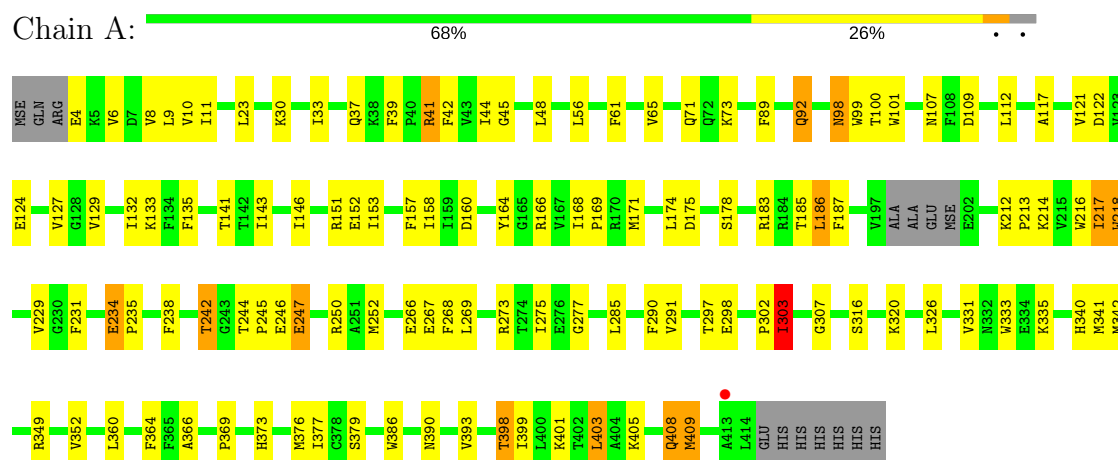
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	0
			125	125		
3	B	139	Total	O	0	0
			139	139		
3	C	119	Total	O	0	0
			119	119		
3	D	81	Total	O	0	0
			81	81		
3	E	148	Total	O	0	0
			148	148		
3	F	99	Total	O	0	0
			99	99		
3	G	89	Total	O	0	0
			89	89		
3	H	113	Total	O	0	0
			113	113		

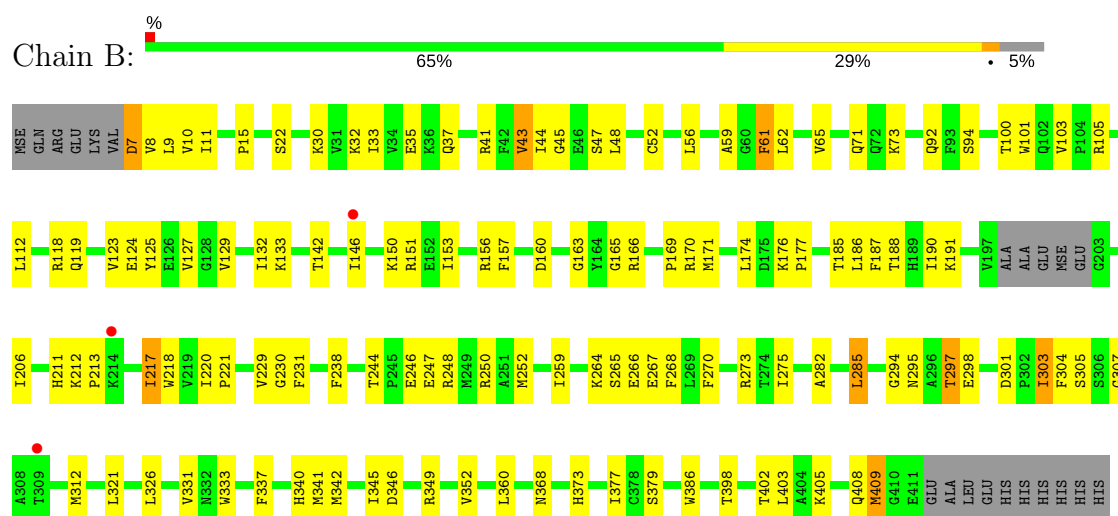
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Flavoprotein/dehydrogenase



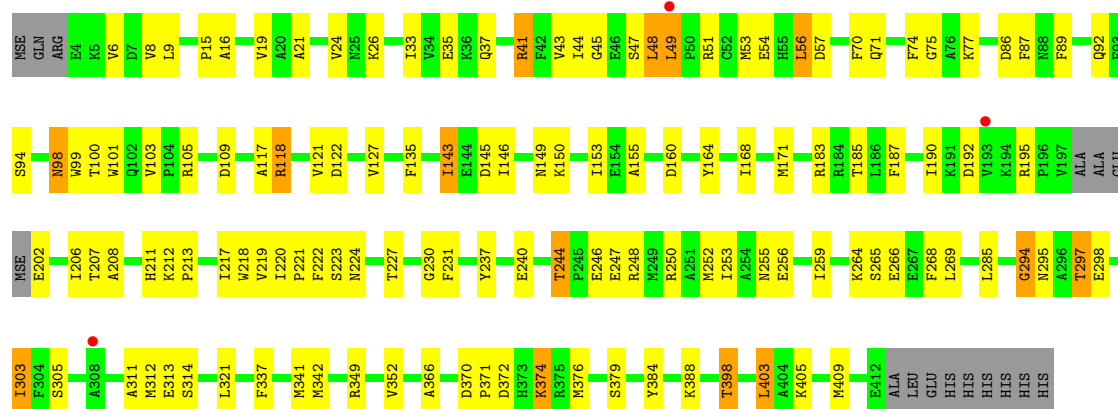
#### • Molecule 1: Flavoprotein/dehydrogenase



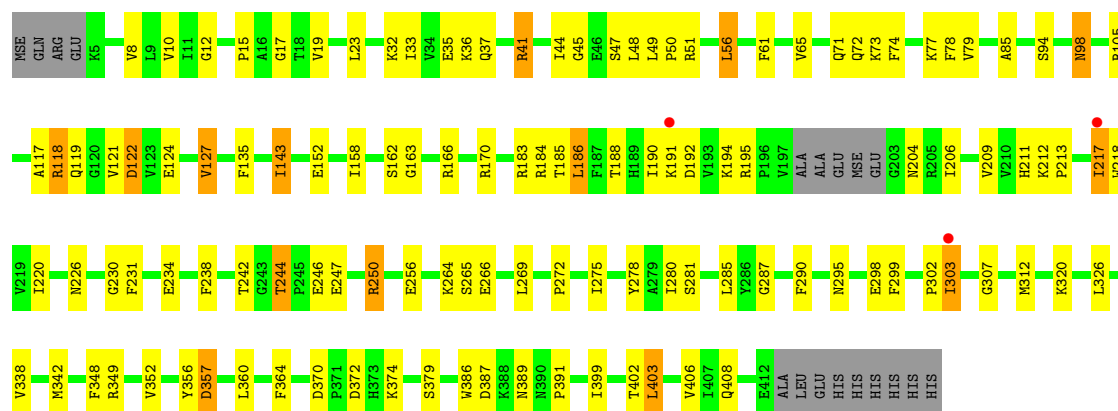
#### • Molecule 1: Flavoprotein/dehydrogenase



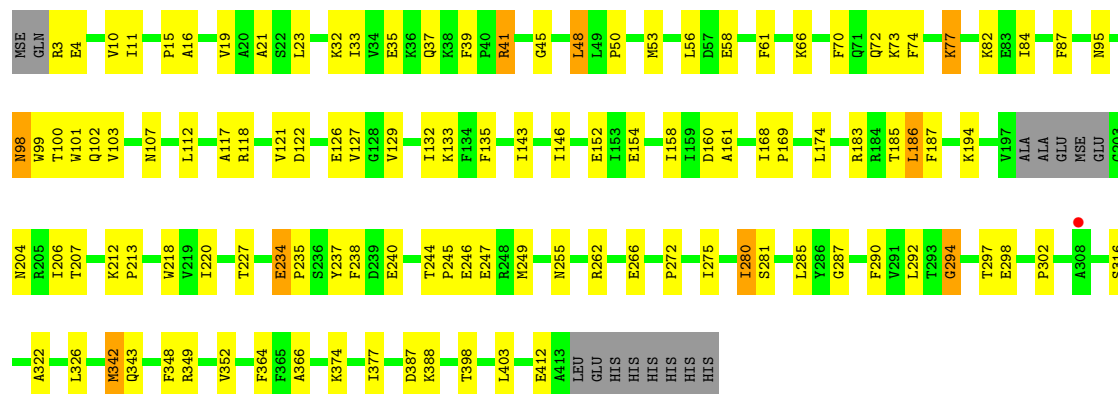




• Molecule 1: Flavoprotein/dehydrogenase



• Molecule 1: Flavoprotein/dehydrogenase



• Molecule 1: Flavoprotein/dehydrogenase





F325	L326	K335	D336	F337	V338	E339	K342	I345	F348	R349	V352	I360	A366	K367	N368	P369	D370	F371	D372	H373	K374	S379	D387	T398	I399	L403	I407	Q408	E411	E412	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.22Å 244.05Å 100.22Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	29.33 – 2.60 29.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.33-2.60) 97.5 (29.73-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, $R_{free}$	0.237 , 0.264 0.227 , 0.255	Depositor DCC
$R_{free}$ test set	5989 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.29 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3396e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	2/3281 (0.1%)	0.64	1/4415 (0.0%)
1	B	0.59	1/3233 (0.0%)	0.63	0/4349
1	C	0.53	1/3256 (0.0%)	0.62	0/4382
1	D	0.44	0/3254	0.59	0/4377
1	E	0.49	0/3283	0.64	0/4415
1	F	0.45	0/3253	0.59	1/4375 (0.0%)
1	G	0.46	0/3275	0.59	0/4406
1	H	0.50	0/3248	0.60	0/4370
All	All	0.50	4/26083 (0.0%)	0.61	2/35089 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	208	ALA	C-N	-5.91	1.20	1.34
1	A	247	GLU	CD-OE2	-5.64	1.19	1.25
1	B	61	PHE	CD2-CE2	-5.37	1.28	1.39
1	A	247	GLU	CD-OE1	-5.09	1.20	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ILE	CB-CA-C	-5.52	100.55	111.60
1	F	96	GLY	N-CA-C	-5.36	99.69	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3210	0	3125	109	0
1	B	3162	0	3084	111	0
1	C	3185	0	3096	111	0
1	D	3183	0	3108	104	0
1	E	3212	0	3136	91	0
1	F	3182	0	3110	120	0
1	G	3204	0	3121	124	0
1	H	3177	0	3090	101	0
2	A	53	0	28	4	0
2	B	53	0	29	5	0
2	C	53	0	29	3	0
2	D	53	0	29	8	0
2	E	53	0	29	5	0
2	F	53	0	28	6	0
2	G	53	0	29	13	0
2	H	53	0	29	10	0
3	A	125	0	0	12	0
3	B	139	0	0	7	0
3	C	119	0	0	5	0
3	D	81	0	0	6	0
3	E	148	0	0	15	0
3	F	99	0	0	14	0
3	G	89	0	0	9	0
3	H	113	0	0	5	0
All	All	26852	0	25100	865	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 865 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:THR:HG22	1:C:298:GLU:H	1.12	1.11
1:D:41:ARG:HH11	1:D:41:ARG:HG2	0.88	1.02
1:B:297:THR:HG22	1:B:298:GLU:H	1.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LEU:HG	3:D:1156:HOH:O	1.58	1.01
1:E:41:ARG:HH11	1:E:41:ARG:HG2	0.87	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/421 (96%)	380 (94%)	22 (6%)	1 (0%)	51	76
1	B	396/421 (94%)	377 (95%)	19 (5%)	0	100	100
1	C	401/421 (95%)	380 (95%)	20 (5%)	1 (0%)	51	76
1	D	399/421 (95%)	378 (95%)	21 (5%)	0	100	100
1	E	402/421 (96%)	387 (96%)	14 (4%)	1 (0%)	51	76
1	F	398/421 (94%)	380 (96%)	18 (4%)	0	100	100
1	G	402/421 (96%)	377 (94%)	24 (6%)	1 (0%)	51	76
1	H	399/421 (95%)	381 (96%)	18 (4%)	0	100	100
All	All	3200/3368 (95%)	3040 (95%)	156 (5%)	4 (0%)	55	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	294	GLY
1	G	210	VAL
1	A	303	ILE
1	E	294	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/340 (99%)	317 (94%)	19 (6%)	24	47
1	B	332/340 (98%)	314 (95%)	18 (5%)	26	49
1	C	332/340 (98%)	315 (95%)	17 (5%)	28	52
1	D	334/340 (98%)	313 (94%)	21 (6%)	21	42
1	E	337/340 (99%)	320 (95%)	17 (5%)	28	53
1	F	335/340 (98%)	318 (95%)	17 (5%)	28	52
1	G	335/340 (98%)	318 (95%)	17 (5%)	28	52
1	H	332/340 (98%)	317 (96%)	15 (4%)	32	59
All	All	2673/2720 (98%)	2532 (95%)	141 (5%)	26	50

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	186	LEU
1	E	56	LEU
1	H	62	LEU
1	D	234	GLU
1	D	357	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	98	ASN
1	F	37	GLN
1	H	71	GLN
1	E	119	GLN
1	E	255	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FAD	A	501	-	51,58,58	2.14	10 (19%)	54,89,89	2.21	17 (31%)
2	FAD	B	502	-	51,58,58	2.19	10 (19%)	54,89,89	2.22	17 (31%)
2	FAD	C	503	-	51,58,58	2.21	13 (25%)	54,89,89	2.35	16 (29%)
2	FAD	D	504	-	51,58,58	2.13	11 (21%)	54,89,89	2.01	11 (20%)
2	FAD	E	505	-	51,58,58	2.09	10 (19%)	54,89,89	2.23	14 (25%)
2	FAD	F	506	-	51,58,58	2.14	8 (15%)	54,89,89	2.04	14 (25%)
2	FAD	G	507	-	51,58,58	2.16	10 (19%)	54,89,89	2.02	12 (22%)
2	FAD	H	508	-	51,58,58	2.16	12 (23%)	54,89,89	2.14	15 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	501	-	-	0/28/50/50	0/6/6/6
2	FAD	B	502	-	-	0/28/50/50	0/6/6/6
2	FAD	C	503	-	-	0/28/50/50	0/6/6/6
2	FAD	D	504	-	-	0/28/50/50	0/6/6/6
2	FAD	E	505	-	-	0/28/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	F	506	-	1/1/9/9	0/28/50/50	0/6/6/6
2	FAD	G	507	-	1/1/9/9	0/28/50/50	0/6/6/6
2	FAD	H	508	-	-	0/28/50/50	0/6/6/6

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	507	FAD	O2'-C2'	-6.59	1.28	1.43
2	F	506	FAD	O2'-C2'	-6.58	1.28	1.43
2	D	504	FAD	O2'-C2'	-6.54	1.29	1.43
2	C	503	FAD	O2'-C2'	-6.54	1.29	1.43
2	B	502	FAD	O2'-C2'	-6.45	1.29	1.43

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	FAD	N3A-C2A-N1A	-9.26	120.80	128.86
2	E	505	FAD	N3A-C2A-N1A	-7.70	122.15	128.86
2	D	504	FAD	N3A-C2A-N1A	-7.69	122.16	128.86
2	B	502	FAD	N3A-C2A-N1A	-7.49	122.34	128.86
2	H	508	FAD	N3A-C2A-N1A	-7.22	122.57	128.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	507	FAD	C2'
2	F	506	FAD	C2'

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	4	0
2	B	502	FAD	5	0
2	C	503	FAD	3	0
2	D	504	FAD	8	0
2	E	505	FAD	5	0
2	F	506	FAD	6	0
2	G	507	FAD	13	0
2	H	508	FAD	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	398/421 (94%)	-0.31	1 (0%) 93 93	10, 26, 48, 62	0
1	B	391/421 (92%)	-0.26	3 (0%) 86 83	14, 29, 50, 65	0
1	C	396/421 (94%)	-0.23	3 (0%) 86 83	13, 29, 51, 66	0
1	D	394/421 (93%)	-0.26	3 (0%) 86 83	12, 31, 51, 71	0
1	E	397/421 (94%)	-0.26	1 (0%) 93 93	11, 26, 46, 64	0
1	F	393/421 (93%)	-0.18	3 (0%) 86 83	16, 31, 52, 71	0
1	G	397/421 (94%)	-0.10	9 (2%) 61 54	15, 33, 63, 78	0
1	H	394/421 (93%)	-0.18	5 (1%) 77 73	18, 33, 51, 65	0
All	All	3160/3368 (93%)	-0.22	28 (0%) 84 81	10, 30, 52, 78	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	GLY	5.1
1	G	278	TYR	4.8
1	G	179	GLY	4.3
1	G	177	PRO	3.5
1	G	280	ILE	3.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FAD	G	507	53/53	0.87	0.23	0.55	31,50,64,82	0
2	FAD	E	505	53/53	0.94	0.16	-0.11	7,23,34,39	0
2	FAD	B	502	53/53	0.95	0.16	-0.12	3,18,35,63	0
2	FAD	H	508	53/53	0.94	0.17	-0.20	12,28,38,48	0
2	FAD	C	503	53/53	0.94	0.16	-0.31	6,20,36,48	0
2	FAD	D	504	53/53	0.93	0.16	-0.36	14,29,42,54	0
2	FAD	F	506	53/53	0.92	0.15	-0.53	16,33,51,85	0
2	FAD	A	501	53/53	0.96	0.13	-0.80	5,19,30,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.